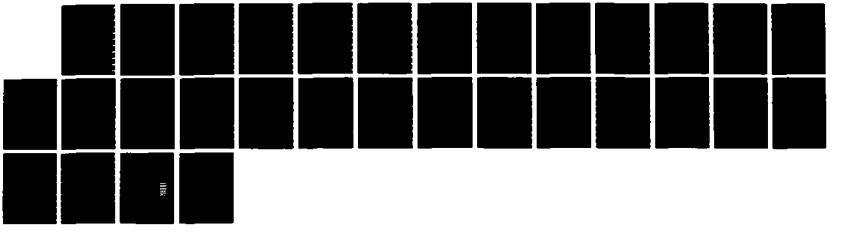
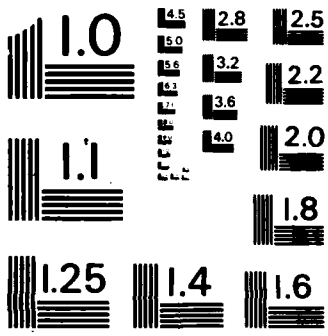
AD-A171 006 EFFICIENT PROCEDURES FOR SOLVING INTEGRAL EQUATIONS 1/1
USED DURING MONTE CAR..(U) ARMY BALLISTIC RESEARCH LAB
ABERDEEN PROVING GROUND MD W B BEVERLY JUL 86
UNCLASSIFIED BRL-MR-3529 F/G 20/8 NL





MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS - 1963 - A

AD-A171 086

AD

US ARMY MATERIEL COMMAND

MEMORANDUM REPORT BRL-MR-3529

EFFICIENT PROCEDURES FOR SOLVING INTEGRAL EQUATIONS USED DURING MONTE CARLO PHOTON-ELECTRON TRANSPORT CALCULATIONS

William B. Beverly

July 1986

DTIC FILE COPY

DTIC ELECTE AUG 1 9 1986 S D E

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

US ARMY BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

86 8 19 035

Destroy this report when it is no longer needed.
Do not return it to the originator.

Additional copies of this report may be obtained from the National Technical Information Service, U. S. Department of Commerce, Springfield, Virginia 22161.

The findings in this report are not to be construed as an official Department of the Army position, unless so designated by other authorized documents.

The use of trade names or manufacturers' names in this report does not constitute indorsement of any commercial product.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER: MEMORANDUM REPORT BRL-MR-3529	2. GOVT ACCESSION NO.: AD-A171086
3. RECIPIENT'S CATALOG NUMBER	
4. TITLE (and Subtitle): EFFICIENT PROCEDURES FOR SOLVING INTEGRAL EQUATIONS USED DURING MONTE CARLO PHOTON-ELECTRON TRANSPORT CALCULATIONS	5. TYPE OF REPORT & PERIOD COVERED
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): William B. Beverly	8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS: US Army Ballistic Research laboratory ATTN: SLCBR-SE Aberdeen Proving Ground, MD 21005-5066	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: 1L1626LAH80
11. CONTROLLING OFFICE NAME AND ADDRESS: US Army Ballistic Research Laboratory ATTN: SLCBR-DD-T Aberdeen Proving Ground, MD 21005-5066	12. REPORT DATE: July 1986 13. NUMBER OF PAGES: 28
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)	15. SECURITY CLASS. (of this report) 15a. DECLASSIFICATION DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release. Distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Integral Equations
Electron Catastrophic Interaction
Collisional Stopping Power
Bremsstrahlung Radiation
Electron-Electron Scattering

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) (idk)

The energy at which electrons and positrons radiate bremsstrahlung photons and their average energy loss when traveling a known distance in a material are derived in Monte Carlo transport studies by solving integral equations. Iterative procedures which use Newton's Method for finding the zero of a function are applied here to efficiently calculate these zeroes. The answers are generally calculated to a high accuracy after four or five iterations. Example calculations are provided and the results are discussed.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

TABLE OF CONTENTS

Page No.

LIST OF FIGURES.....5

I. INTRODUCTION.....7

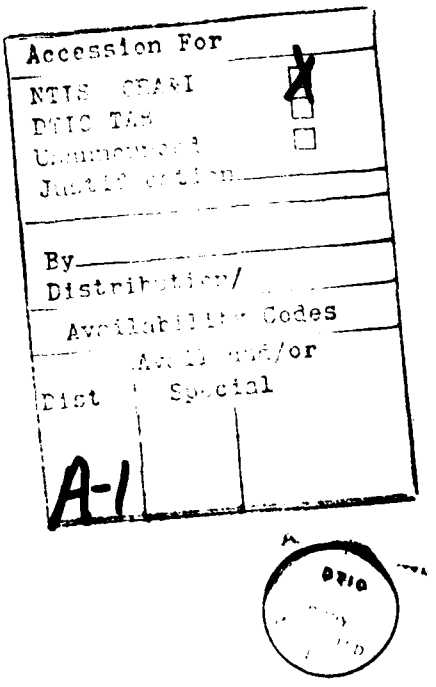
II. THE SOLUTION PROCEDURES.....9

III. EXAMPLE SOLUTIONS OF THE TWO INTEGRAL EQUATIONS.....17

IV. CONCLUSIONS AND PROGNOSIS.....25

V. REFERENCES.....26

DISTRIBUTION LIST.....27



LIST OF FIGURES

Figure No. Page No.

1. The Linear Approximation of $\epsilon(T)$ Used To Derive a First Estimate of T_s in the Mass-Range Problem.....11

2. The Linear Approximation of $\sigma(T)/\epsilon(T) = g(T)$ Used To Derive a First Estimate of T_s in the Catastrophic Sampling Problem.....14

3. The Linear Approximation of $\epsilon(T)$ Applied to the Example Mass-Range Problem.....19

4. The Linear Approximation of $\sigma(T)/\epsilon(T) = g(T)$ Applied to the Example Catastrophic Sampling Problem.....22

I. INTRODUCTION

A Monte Carlo computer program EDPEC[1] has been constructed at the Ballistic Research Laboratory to calculate, as a function of mass depth along the beam axis, the local energy deposition by an electron beam and its associated secondary electrons and positrons. Since the distributional accuracy of calculations using such Monte Carlo procedures varies as $1/\sqrt{N}$, where N is the number of sample cascades,[2] efficient calculational procedures are generally needed to keep the calculational times at an acceptable level when high accuracies are required of the answers.

In this connection, the integral equations,

$$u(T_0, T_u) = \int_{T_u}^{T_0} \frac{dT}{\epsilon(T)} , \tag{1}$$

and

$$1 - e^{-\int_{T_u}^{T_0} \frac{\sigma(T)}{\epsilon(T)} dT} = RM(0,1) , \tag{2}$$

are frequently solved to find respectively the average energy $(T_0 - T_u)$ lost by an electron or positron which has traveled a known mass distance u and the kinetic energy T_u at which a catastrophic electronic interaction occurs. The quantity T_0 in the preceding equations is the initial kinetic energy of an electron, T_u is the average residual kinetic energy of an electron which has traveled a mass distance $u(T_0, T_u)$, and $RM(0,1)$ is a random number picked with equal probability at any point in the range from 0 to 1. A catastrophic interaction is identified here as either a radiative transition in which a bremsstrahlung photon with energy greater than 0.1-MeV is emitted or an electron-electron scattering in which a knock-on electron having energy greater than 0.1-MeV is ejected.

---

[1]W.B. Beverly, "EDPEC: A Computer Program for Calculating the Energy Deposition by an Photon-Electron Cascade in Multi-Slab Arrays," In Publication as a BRL Technical Report.

[2]Y.U. Shreider, The Monte Carlo Method, The Method of Statistical Trials, Pergamon Press, Aylesbury, Bucks, Great Britain, 1967.

The quantity $\epsilon(T)$ is the restricted stopping power[3] (MeV-cm^2/g) of electrons and positrons in a material, and $\sigma(T)$ is the mass cross section (cm^2/g) for bremsstrahlung production. All functions used in the preceding equations are derived by piecewise fitting tabular data to interpolation functions tractable for calculations of the type described in this report. Since a significant fraction of the total calculational effort of EDPEC is expended on evaluating these integrals, an increase in the associated calculational efficiency would be expected to significantly reduce the overall calculational effort.

These integral equations were initially solved using the bisection method[4] where about twenty iterations were generally needed to reduce the interval enclosing an answer to 0.0001 percent of its initial width. However, since the calculational times for problems of interest turned out to be very long, an attempt was made to find more efficient procedures. We describe such procedures, which are derived by applying Newton's Method[4] for finding the zero of an analytic function, in the next section of this report. Example calculations, where tractable analytic functions are substituted for $\epsilon(T)$ in Equation 1 and $\sigma(T)/\epsilon(T)$ in Equation 2, are described in Section III.

---

[3]M.J. Berger and S.H. Seltzer, "Stopping Powers and Ranges of Electrons and Positrons (2nd Ed.)," Prepared for: U.S. Department of Commerce, Office of Health and Environmental Research, Office of Naval Research. NBSIR 82-2550-A, December 1982.

[4]S.D. Conte and C. deBoor, ELEMENTARY NUMERICAL ANALYSIS, An Algorithmic Approach, McGraw-Hill Book Company, Third Edition (1980).

II. THE SOLUTION PROCEDURES

An improved estimate x_z^{i+1} of the location x_z of a zero of the equation

$$F(x) = 0 \tag{3}$$

can be derived from an estimate x_z^i by using Newton's Method[4], that is

$$x_z^{i+1} = x_z^i - \frac{F(x_z^i)}{F'(x_z^i)}, \tag{4}$$

if the first derivative $F'(x_z^i)$ is continuous and non-zero between x_z^i and x_z. The application of this method to the aforementioned EDPEC integral equations will now be described.

The electron-range problem as developed in EDPEC is defined in the following manner:

1. An electron having an initial kinetic energy T_0 travels a known mass distance $u(T_0, T_u)$ while constantly losing energy. The unknown residual kinetic energy, known to lie between T_0 and T_1, is obtained by solving Equation 1,

$$u(T_0, T_u) = \int_{T_u}^{T_0} \frac{dT}{\epsilon(T)}. \tag{1}$$

The range of validity of a fitted interpolation function extends from T_0 down to T_1. Since the form of $\epsilon(T)$ used by EDPEC does not permit the indefinite integral $\int \frac{dT}{\epsilon(T)}$ to be expressed in a closed form, any associated definite integral is evaluated by expanding the integrand in a convergent series. Consequently, the definite integral $\int_{T_1}^{T_0} \frac{dT}{\epsilon(T)}$ and any intermediate definite integral whose lower limit lies between T_0 and T_1 can be approximated to any specified accuracy by evaluating a sufficient number of terms.

2. The electron mass range integral (Equation 1) can be rearranged to the form of Equation 3, that is

$$F(T_u) = \int_{T_u}^{T_0} \frac{dT}{\epsilon(T)} - u(T_0, T_u) = 0. \tag{5A}$$

The first derivative, needed in the Newtonian iteration formula, is

$$\frac{d}{dT_u}[F(T_u)] = F'(T_u) = -\frac{1}{\epsilon(T_u)}, \tag{5B}$$

since T_0 and $u(T_0, T_u)$ are known in the problems being discussed and T_u is the unknown quantity.

3. The derivative of $F(T)$ is non-zero on the range from T_0 to T_1 since $\epsilon(T)$ is positive and non-zero. Consequently, Newton's Method may be applied to calculate a better approximation T_u^{i+1} from any estimate T_u^i which lies between T_0 and T_1.

4. The mass distance, $u(T_0, T_1) = \int_{T_1}^{T_0} \frac{dT}{\epsilon(T)}$, as well as the associated indefinite integrals, have been calculated earlier, and these values can be retrieved and used in further calculations such as the derivation of an initial estimate T_u^i of T_u.

5. The value of any element in the set of quantities, $[T_s^i, \epsilon(T_s^i), F(T_s^i), F'(T_s^i), u(T_0, T_s^i)]$, needed during the calculation of a first or improved estimate, has been or can be easily calculated.

Item 5 completes the definition of the electron-range integral-equation problem. A first estimate T_u^1 is derived by assuming that the stopping power between T_0 and T_1 is approximated by the linear relation $\epsilon^\dagger(T)$ whose slope m is derived from the points, $[T_0, \epsilon(T_0)]$ and $[T_1, \epsilon(T_1)]$ (Figure 1), that is

$$m = \frac{\epsilon(T_0) - \epsilon(T_1)}{T_0 - T_1}. \tag{6A}$$

The function $\epsilon^\dagger(T)$ is then derived by translating the points, $[T_0, \epsilon(T_0)]$ and $[T_1, \epsilon(T_1)]$, a distance $\Delta\epsilon$ so that the mass distance $u^\dagger(T_0, T_1)$, calculated using $\epsilon^\dagger(T)$, is equal to $u(T_0, T_1)$, that is

$$u^\dagger(T_0, T_1) = \int_{T_1}^{T_0} \frac{dT}{\epsilon^\dagger(T)} = \int_{T_1}^{T_0} \frac{dT}{m(T - T_1) + \epsilon(T_1) + \Delta\epsilon} = u(T_0, T_1). \tag{6B}$$

The magnitude of the translation is derived to be

$$\Delta\epsilon = \frac{\epsilon(T_1)\, e^{m\, u(T_0, T_1)} - m\,(T_0 - T_1) - \epsilon(T_1)}{1 - e^{m\, u(T_0, T_1)}}, \tag{6C}$$

and the linear equation $\epsilon^\dagger(T)$ is given by

$$\epsilon^\dagger(T) = m\,(T - T_1) + \epsilon(T_1) + \Delta\epsilon. \tag{6D}$$

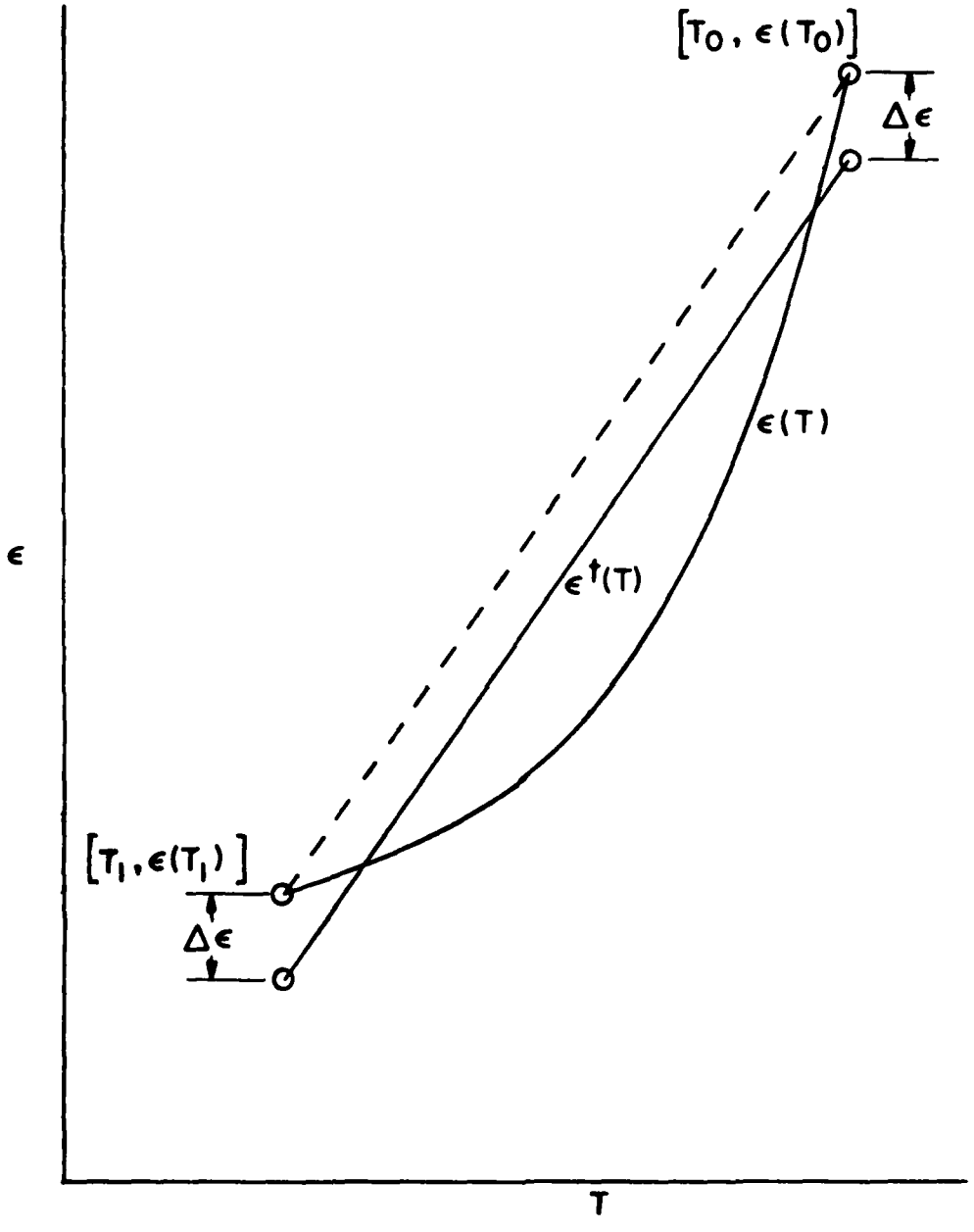


Figure 1. The Linear Approximation of $\epsilon(T)$ Used To Derive a First Estimate of T_* in the Mass-Range Problem.

The value of the first estimate T_u^1 of the residual energy of an electron which has traveled a known mass distance $u(T_0, T_u)$ is then calculated by solving the integral equation

$$\int_{T_u^1}^{T_0} \frac{dT}{m(T - T_1) + \epsilon(T_1) + \Delta\epsilon} = u(T_0, T_u) . \tag{6E}$$

This is found to be

$$T_u^1 = T_1 - \frac{1}{m}\left[\epsilon(T_1) + \Delta\epsilon - e^{-m\,u(T_0,T_1)}\left(m(T_0 - T_1) + \epsilon(T_1) + \Delta\epsilon\right)\right] . \tag{6F}$$

Finally, the first estimate just calculated is iteratively improved using Equation 4 until a specified accuracy has been attained.

The first estimate as derived above has proved in practice to be sufficiently accurate so that subsequent iterations rapidly converged toward the true answer. In general, three or four iterations are sufficient to attain an accuracy well within the overall EDPEC calculational accuracy.

The catastrophic sampling problem as developed in EDPEC is defined in the following manner:

1. An electron having an initial kinetic energy T_0 loses energy continuously as it travels through a medium until it suffers a catastrophic interaction during which a finite amount of energy is instantaneously lost. The kinetic energy of an electron as it enters into a catastrophic interaction is obtained by solving Equation 2,

$$1 - e^{-\int_{T_s}^{T_0} \frac{\sigma(T)}{\epsilon(T)}\,dT} = RN(0,1) , \tag{2}$$

where T_s is known to lie between T_0 and T_1. The mass cross sections for catastrophic interactions are also piecewise fitted on the interval from T_0 to T_1 by functions $\sigma(T)$ which are tractable to sampling calculations of the type discussed in this report. As described earlier in Item 1 of the mass-range-problem description, the integrals associated with Equation 2 cannot be given in closed form. Consequently, the definite integral $\int_{T_1}^{T_0} \frac{\sigma(T)}{\epsilon(T)}\,dT$ and any intermediate definite integral whose lower limit lies between T_0 and T_1 are evaluated to an acceptable accuracy by summing a sufficient number of terms of a convergent series expansion.

2. The catastrophic sampling integral, (Equation 2) can be rearranged to the form of Equation 3, that is

$$F(T_s) = 1 - e^{-\int_{T_s}^{T_0} \frac{\sigma(T)}{\epsilon(T)}\,dT} - RN(0,1) = 1 - e^{-c(T_s,T_0)} - RN(0,1) = 0 . \quad (7A)$$

The first derivative $F'(T_s)$ of $F(T_s)$, needed by Newton's iteration formula, is

$$\frac{dF(T_s)}{dT} = F'(T_s) = \left[e^{-\int_{T_s}^{T_0} \frac{\sigma(T)}{\epsilon(T)}\,dT} \right] \left[\frac{\sigma(T_s)}{\epsilon(T_s)} \right] . \quad (7B)$$

since T_0 and $RN(0,1)$ are known constants.

3. Since the functions, $\sigma(T)$ and $\epsilon(T)$, are positive and non-zero between T_0 and T_1, the function $F'(T)$ does not vanish. Consequently, Newton's Method may be applied to calculate a better approximation T_s^{i+1} when T_s^i lies between T_0 and T_1.

4. The definite integral, $\int_{T_1}^{T_0} \frac{\sigma(T)}{\epsilon(T)}\,dT = c(T_0,T_1)$, along with the associated indefinite integrals at T_0 and T_1, have been calculated earlier and can be retrieved for subsequent calculations such as the derivation of an initial estimate T_s^1 of T_s. For calculational convenience, $g(T) = \sigma(T)/\epsilon(T)$ in the following discussion.

5. The value of any element in the set, $[T_s^i, g(T_s^i), F(T_s^i), F'(T_s^i), c(T_0,T_s)]$ between T_0 and T_1 has been or can be easily calculated during the derivation of an initial estimate or the conduction of subsequent iterations.

Item 5 completes the definition of the catastrophic-sampling integral-equation problem. A first estimate T_s^1 of the solution of Equation 7A is derived by approximating the function $g(T) = \sigma(T)/\epsilon(T)$ by the more tractable linear relation $g^\dagger(T)$. One point on $g^\dagger(T)$ is constrained to pass through the point $[T_0, g(T_0)]$ (Figure 2), and the approximation integral $c^\dagger(T_0,T_1)$ is set equal to the true integral, that is

$$c^\dagger(T_0,T_1) = \int_{T_1}^{T_0} g^\dagger(T)\,dT = c(T_0,T_1) = \int_{T_1}^{T_0} \frac{\sigma(T)}{\epsilon(T)}\,dT . \quad (8A)$$

Performing the rotation about T_0 as described, the value of g at T_1 is

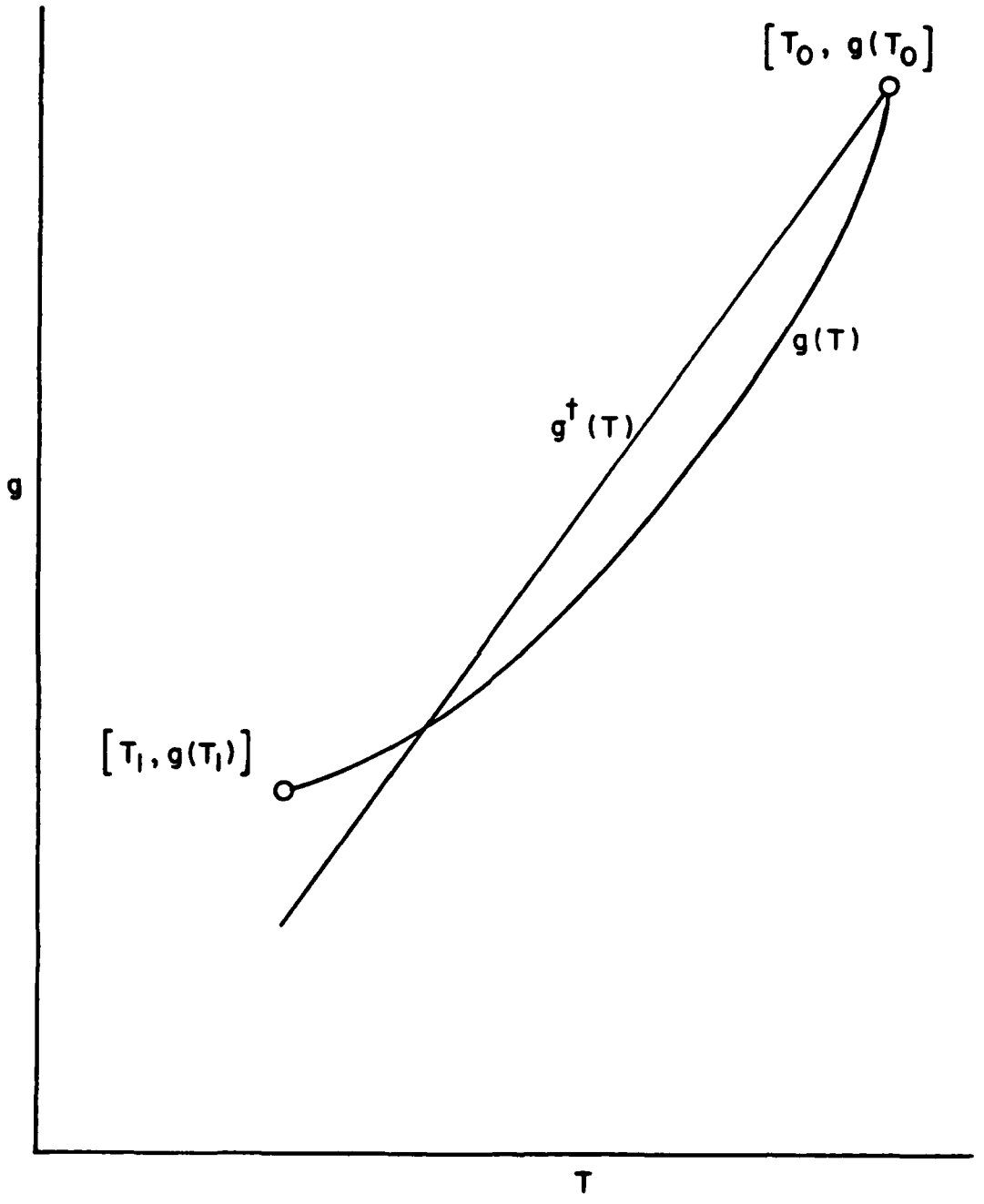


Figure 2. The Linear Approximation of $\sigma(T)/\epsilon(T) = g(T)$ Used To Derive a First Estimate of T_s in the Catastrophic Sampling Problem.

derived to be

$$g^{\dagger}(T_1) = \frac{2\,[c(T_0,T_1)]}{T_0 - T_1} - g(T_0)\,. \tag{8B}$$

The linear approximation of $g(T)$ from T_0 to T_1 becomes

$$g^{\dagger}(T) = m\,(T - T_0) + g(T_0) \tag{8C}$$

whose slope m is

$$m = \frac{g(T_0) - g^{\dagger}(T_1)}{T_0 - T_1}\,. \tag{8D}$$

The first estimate T_s^1 of T_s is now derived by solving the integral equation

$$e^{-c^{\dagger}(T_0,T_s^1)} = 1 - RN(0,1) \tag{8E}$$

which can be changed to

$$\int_{T_s^1}^{T_0} [m\,(T - T_0) + g(T_0)]\,dT = -\ln[1 - RN(0,1)]\,. \tag{8F}$$

This reduces to the quadratic equation

$$(T_s^1)^2 - 2\,[T_0 - \frac{g(T_0)}{m}\,]\,(T_s^1) + T_0^2 - \frac{2}{m}\ln[1 - RN(0,1)] - \frac{2\,g(T_0)\,T_0}{m} = 0 \tag{8G}$$

of the variable T_s^1 whose solutions are the well known

$$(T_s^1) = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

where:

$$a = 1$$

$$b = -2\left[T_0 - \frac{g(T_0)}{m}\right],$$

and

$$c = T_0^2 - \frac{2}{m}\ln[1 - RN(0,1)] - \frac{2 \times g(T_0) \times T_0}{m}\,.$$

It is noted without explanation that Equation 8G is never solved in EDPEC for $RN(0,1) = 1$ so that the infinity of $\ln(0)$ never occurs in practice. The appropriate solution to the problem at hand is selected from the two

available solutions as that solution which lies between T_0 and T_1. This estimate is iteratively improved using Newton's Method until an acceptable accuracy has been attained.

The first estimate as derived above has proved to be quite close to the true answer for a test problem whose solution is illustrated later in Section III of this report. Four or five subsequent iterations generally proved sufficient to provide an acceptable accuracy when this first estimate was inserted into Newton's Procedure (Equation 4).

III. EXAMPLE SOLUTIONS OF THE TWO INTEGRAL EQUATIONS

Tractable functions were selected in turn for $\overline{T}/\epsilon(T)$ (Equation 1) and $\sigma(T)/\epsilon(T) = g(T)$ (Equation 2) which are illustrative of the behavior of these functions over the electron energy ranges of interest. Example problems were devised using these equations and a short computer program was written to solve each problem. The range of values of the dependent variable T was selected for calculational convenience and does not correspond to the kinetic energy (MeV) of the electrons in problems of interest.

The stopping power in the mass-range problem is taken to be

$$\epsilon(T) = 1 + 0.1T^2 . \tag{9A}$$

The initial energy of an electron is taken to be $T = 3$ (Arbitrary Units) and solutions are sought for a range of mass distances up to that associated with a total loss of kinetic energy ($T = 0$). The mass range integral is

$$u(T_0, T_u) = \int_{T_u}^{T_0} \frac{dT}{1 + 0.1T^2} , \tag{9B}$$

and the associated equation to be solved is

$$F(T_u) = \int_{T_u}^{T_0} \frac{dT}{1 + 0.1T^2} - u(T_0, T_u) = 0 , \tag{9C}$$

where T_0 and $u(T_0, T_u)$ are known and T_u is unknown. The derivative $F'(T_u)$ of $F(T_u)$ is

$$F'(T_u) = \frac{d}{dT_u}[F(T_u)] = \frac{-1}{1 + 0.1T_u^2} . \tag{9E}$$

The maximum mass distance traveled by an electron in the specified energy range is identified as

$$u(3,0) = \int_0^3 \frac{dT}{1 + 0.1T^2} , \tag{9F}$$

and can be easily evaluated in closed form.

Solutions of T_u associated with mass depths ranging from the very small to those close to the maximum value of $u(3,0)$ are needed in order to demonstrate whether the developed procedures are effective over the total energy range of a problem. In this connection, solutions are calculated in

turn for depths given by

$$u_n[3,(T_u)_n] = \frac{(n-1)\,u(3,0)}{25},$$

where n ranges in value from 2 to 25 as well as the values,

$$u_1[3,(T_u)_1] = 0.0001,$$

and

$$u_{26}[3,(T_u)_{26}] = u(3,0) - 0.0001.$$

A short computer program was constructed to solve this set of problems. The first step in calculating a solution for a specified mass depth is to derive the linear approximation $\epsilon^1(T)$ of $\epsilon(T)$ (Figure 3). The slope m and translation increment $\Delta\epsilon$ are derived as described by Equations 6A and 6D, respectively. The initial estimate T_e^1 is then calculated using Equation 6F. Finally, the initial estimate is iteratively improved using Newton's Method (Equation 4) until a specified accuracy has been attained.

Representative results from the example calculation are given in Table 1. Convergence is very rapid for each problem in the set; three iterations after the first estimate are sufficient in all cases to obtain a very good accuracy.

The integrand $g(T)$ associated with the catastrophic sampling problem is taken to be

$$g(T) = \frac{\sigma(T)}{\epsilon(T)} = T^2 - 3T + 4. \tag{10A}$$

The initial energy of an electron is taken to be 3 (Arbitrary Units), and the transport of the electron is to be conducted until it either suffers a catastrophic interaction or its energy is reduced to 1. The catastrophic sampling equation is

$$1 - e^{-c(T_0,T_e)} = RN(0,1) \tag{10B}$$

where

$$c(T_0,T_e) = \int_{T_e}^{T_0} \frac{\sigma(T)}{\epsilon(T)}\,dT = \int_{T_e}^{T_1} g(T)\,dT = \int_{T_e}^{T_0} (T^2 - 3T + 4)\,dT. \tag{10C}$$

The associated equation to be solved is

$$F(T_e) = 1 - RN(0,1) - e^{-c(T_0,T_e)} = 0 \tag{10D}$$

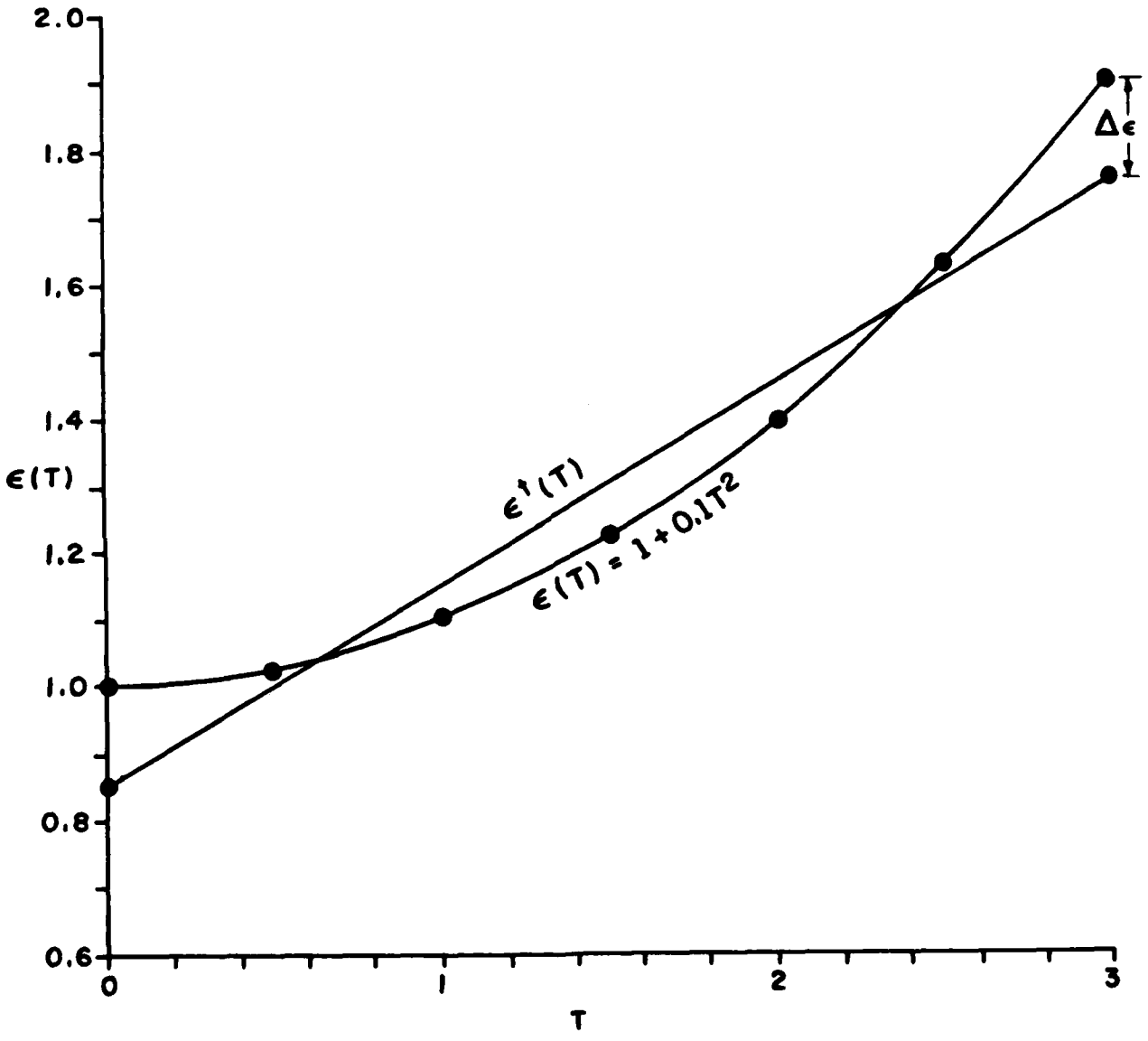


Figure 3. The Linear Approximation of $\epsilon(T)$ Applied to the Example Mass-Range Problem.

u(3,0) = 2.4003907652633		$\Delta\epsilon$ = -0.1466557965344	
I	T_u^I	$F(T_u^I)$	ΔT_u^I
	n = 1	u(3,T) = 0.0000100000000	
1	2.9999824665843	-0.0000007718609	0.0000014665276
2	2.9999810000567	0.0000000000002	-0.0000000000003
3	2.9999810000570	-0.0000000000000	0.0000000000000
	n = 5	u(3,T) = 0.3840625224421	
1	2.3639520227107	-0.0136311085117	0.0212485388507
2	2.3427034838600	0.0000439806607	-0.0000681183890
3	2.3427716022490	0.0000000004531	-0.0000000007019
4	2.3427716029509	-0.0000000000000	0.0000000000000
	n = 10	u(3,T) = 0.8641406754948	
1	1.6653316461874	0.0034329650556	-0.0043850393790
2	1.6697166855663	0.0000019628597	-0.0000025100959
3	1.6697191956623	0.0000000000006	-0.0000000000008
4	1.6697191956631	-0.0000000000000	0.0000000000000
	n = 15	u(3,T) = 1.3442188285475	
1	1.0604190045084	0.0330169617933	-0.0367296810623
2	1.0971486855707	0.0001163822100	-0.0001303915468
3	1.0972790771175	0.0000000014861	-0.0000000016650
4	1.0972790787825	0.0000000000000	0.0000000000000
	n = 20	u(3,T) = 1.8242969816001	
1	0.5366448399415	0.0445132895760	-0.0457952174943
2	0.5824400574357	0.0001089978658	-0.0001126954704
3	0.5825527529061	0.0000000006920	-0.0000000007155
4	0.5825527536216	0.0000000000000	0.0000000000000
	n = 26	u(3,T) = 2.4003807652633	
1	0.0000085334548	0.0000014665452	-0.0000014665452
2	0.0000100000000	0.0000000000000	-0.0000000000000
3	0.0000100000000	0.0000000000000	0.0000000000000

Table 1. Representative Solutions of the Mass-Range Example Problem.

and its derivative $F'(T_s)$ is

$$F'(T_s) = \frac{d}{T_s}F(T_s) = -e^{-c(T_0,T_s)}\frac{d}{dT_s}\left[-c(T_0,T_s)\right] . \qquad (10E)$$

Since the maximum value of the catastrophic sampling integral on this energy range is

$$c(3,1) = \int_1^3 (T^2 - 3T + 4)\, dT = 14/3 , \qquad (10F)$$

then a catastrophic interaction will only occur when the random number lies on the range

$$0 \leq RN(0,1) \leq 1 - e^{-14/3} . \qquad (10G)$$

Solutions of T_s associated with random numbers ranging from those close to 0 to those values close to the maximum value described above in Equation 10G are used in order to demonstrate if the procedures are effective over the total energy range of a problem. In this connection, the random numbers, ordinarily selected using stochastic procedures, are calculated deterministically as

$$RN_n(0,1) = \frac{(n-1)\, RN(0,1 - e^{-14/3})}{25}$$

where n ranges in value from 2 to 25 as well as the values

$$RN_1(0,1) = 0.0001 ,$$

and for

$$RN_{26}(0,1) = 1 - e^{-14/3} - 0.0001 .$$

A short computer program was constructed to solve this set of problems. The first step in calculating a solution for a specified random number is to derive the linear approximation $g^1(T)$ of $g(T)$ (Figure 4). The derivation of the linear approximation used here differs from that described earlier for the mass-range problem in that $g^1(T)$ is derived by rotating $g(T)$ about T_0 until the associated sampling integral $w^1(T_0, T_1)$ is equal to $w(T_0, T_1)$ (Figure 4). This rotation is conducted as described by Equation 8B, and an initial estimate T_s^1 is calculated by solving Equation 8G. Finally, the initial estimate is iteratively improved using Newton's Method until a specified accuracy is obtained.

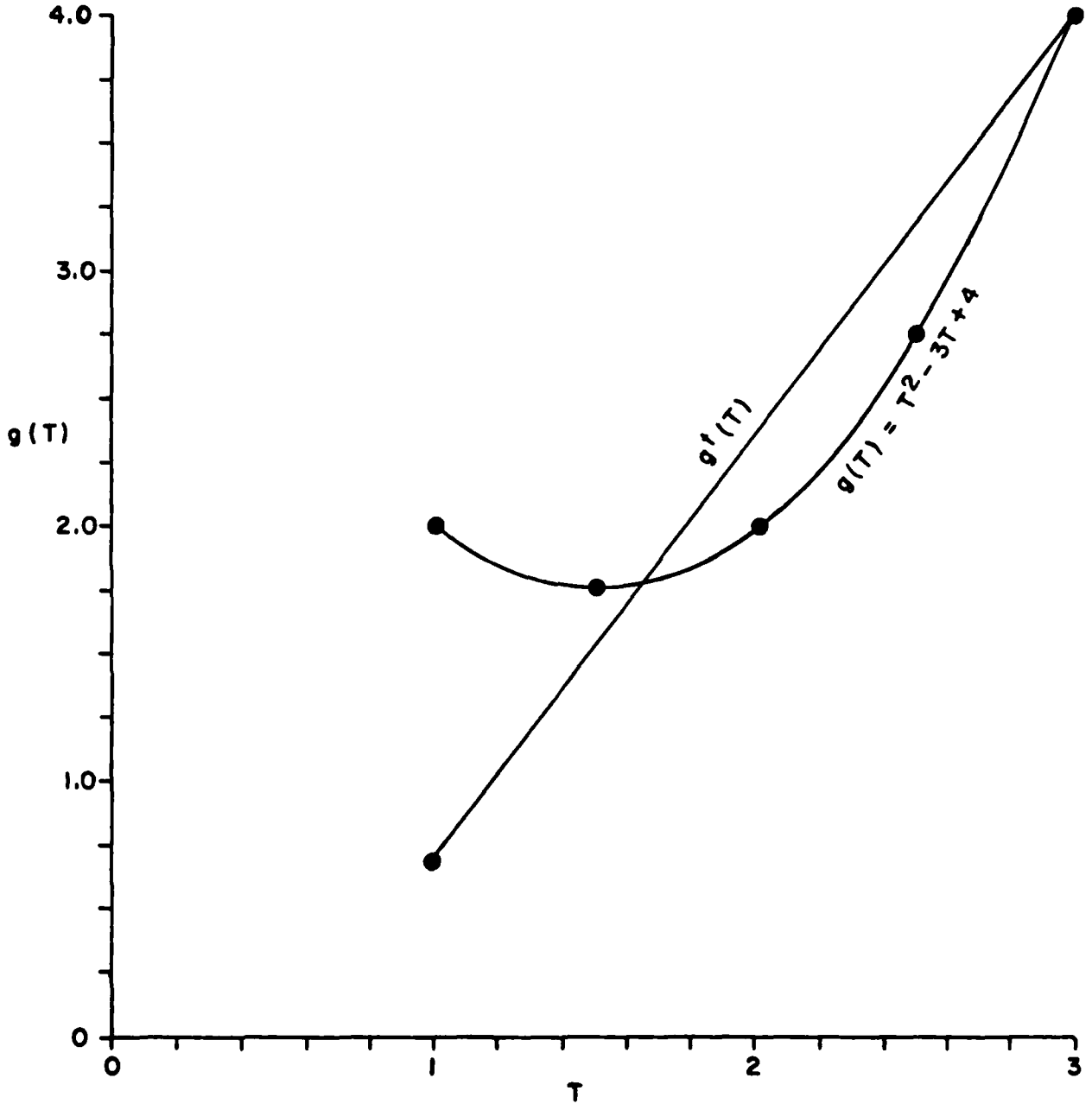


Figure 4. The Linear Approximation of $\sigma(T)/\epsilon(T) = g(T)$ Applied to the Example Catastrophic Sampling Problem.

Representative results are given in Table 2. Convergence is very rapid for all cases; five iterations from initial estimate are sufficient in all cases to obtain a very good accuracy.

$c(3,1) = 4.6666666666667$		$[g^{\dagger}(T)]' = 0.6666666666667$	
I	T_S^I	$F(T_S^I)$	ΔT_S^I
	n = 5	rn = 0.1584952699918	
1	2.9564642213854	-0.0010408024021	0.0003190945754
2	2.9561451268099	-0.0000007673761	0.0000002356134
3	2.9561448911965	-0.0000000000004	0.0000000000001
4	2.9561448911964	-0.0000000000000	0.0000000000000
	n = 20	rn = 0.7528525324609	
1	2.6205632622800	-0.0199883563891	0.0248945802238
2	2.5956686820562	-0.0009004277777	0.0012303231939
3	2.5944383588623	-0.0000020420717	0.0000028029407
4	2.5944355559216	-0.0000000000106	0.0000000000145
5	2.5944355559072	0.0000000000000	-0.0000000000000
	n = 24	rn = 0.9113478024526	
1	2.2888927291901	-0.0215122039163	0.0823122638492
2	2.2065804653409	-0.0024388256425	0.0119032702411
3	2.1946771950998	-0.0000411876600	0.0002080029803
4	2.1944691921195	-0.0000000122261	0.0000000617803
5	2.1944691303393	-0.0000000000000	0.0000000000000
6	2.1944691303393	0.0000000000000	-0.0000000000000
	n = 25	rn = 0.9509716199506	
1	2.0634113718903	-0.0178810679518	0.1292631377944
2	1.9341482340959	-0.0026371822739	0.0263315613811
3	1.9078166727148	-0.0000806562499	0.0008570572678
4	1.9069596154470	-0.0000000808750	0.0000008611080
5	1.9069587543390	-0.0000000000001	0.0000000000009
6	1.9069587543381	-0.0000000000000	0.0000000000000
	n = 26	rn = 0.9905854374485	
1	1.0017498014171	-0.0000219519556	0.0011641557120
2	1.0005856457051	-0.0000000191512	0.0000010173989
3	1.0005846283061	-0.0000000000000	0.0000000000008
4	1.0005846283054	-0.0000000000000	0.0000000000000

Table 2. Representative Solutions of the Catastrophic Sampling Problem.

IV. CONCLUSIONS AND PROGNOSIS

Improved procedures for solving certain integral equations associated with the Monte Carlo simulation of electron-photon cascades have been investigated. The efficiency of these procedures has been illustrated for integral equations where tractable functions, representative of the bremsstrahlung cross sections and the electron stopping power, have been substituted. In fact, these example functions may provide a more strenuous test of the forgoing procedures than the actual functions $\sigma(T)$ and $\epsilon(T)$. Example results are given.

These procedures have been introduced into the photon-electron cascade computer program EDPEC. The calculational times for a fixed number of cascades have been reduced to about 50 percent of those needed when the bisection method was used to solve the integral equations. In this comparison, the accuracy criteria for each case was set to be much higher than the overall calculational accuracy of EDPEC. No error analysis has been conducted to determine if a lesser accuracy (and associated decrease in calculational times) can be used without degrading the overall calculational accuracy of EDPEC.

Smaller improvements in the calculational efficiencies may still be obtainable by devising better procedures for calculating the first estimate of the solution. This possibility will be kept in mind as EDPEC is used in future studies.

V. REFERENCES

1. W.B. Beverly, "EDPEC: A Computer Program for Calculating the Energy Deposition by an Photon-Electron Cascade in Multi-Slab Arrays," In Publication as a BRL Technical Report.

2. Y.U. Shreider, The Monte Carlo Method, The Method of Statistical Trials, Pergamon Press, Aylesbury, Bucks, Great Britain, 1967.

3. M.J. Berger and S.H. Seltzer, "Stopping Powers and Ranges of Electrons and Positrons (2nd Ed.)," Prepared for: U.S. Department of Commerce, Office of Health and Environmental Research, Office of Naval Research. NBSIR 82-2550-A, December 1982.

4. S.D. Conte and C. deBoor, ELEMENTARY NUMERICAL ANALYSIS, An Algorithmic Approach, McGraw-Hill Book Company, Third Edition (1980)

DISTRIBUTION LIST

No. of Copies	Organization
12	Administrator Defense Technical Info Center ATTN: DTIC-DDA Cameron Station Alexandria, VA 22304-6145
1	HQDA DAMA-ART-M Washington, DC 20310
1	Commander US Army Materiel Command ATTN: AMCDRA-ST 5001 Eisenhower Avenue Alexandria, VA 22333-0001
1	Commander Armament R&D Center US Army AMCCOM ATTN: SMCAR-TSS Dover, NJ 07801
1	Commander Armament R&D Center US Army AMCCOM ATTN: SMCAR-TDC Dover, NJ 07801
1	Director Benet Weapons Laboratory Armament R&D Center US Army AMCCOM ATTN: SMCAR-LCB-TL Watervliet, NY 12189
1	Commander US Army, Armament, Munitions & Chemical Command ATTN: SMCAR-ESP-L Rock Island, IL 61299
1	Commander US Army Aviation R&D Command ATTN: AMSAV-E 4300 Goodfellow Blvd St. Louis, MO 63120
1	Director US Army Air Mobility R&D Laboratory Ames Research Center Moffett Field, CA 94035
1	Commander US Army Communications - Electronics Command ATTN: AMSEL-ED Fort Monmouth, NJ 07703
1	Commander ERADCOM Technical Library ATTN: DELSD-L (Reports Section) Fort Monmouth, NJ 07703-5301
1	Commander US Army Missile Command RD&E Cntr ATTN: AMSMI-RD Redstone Arsenal, AL 35898
1	Commander US Army Missile & Space Intelligence Center ATTN: AMSMI-YDL Redstone Arsenal, AL 35898
1	Commander US Army Tank Automotive Command ATTN: AMSTA-TSL Warren, MI 48397-5000
1	Director US Army TRADOC Systems Analysis Activity ATTN: ATAA-SL White Sands Missile Range, NM 88002
1	Commandant US Army Infantry School ATTN: ATSH-CD-CSO-OR Fort Benning, GA 31905
1	Commander US Army Deployment & Employment Agency ATTN: MODE-TED-SAB Fort Lewis, WA 98433

DISTRIBUTION LIST

No. of Copies	Organization
1	Air Force Armament Laboratory ATTN: AFATL/DLODL Eglin AFB, FL 32542-5000
10	Central Intelligence Agency Office of Central Reference Dissemination Branch Room GE-47 HQS Washington, D.C. 20502

No. of Copies	Organization
	Aberdeen Proving Ground
	Dir, USAMSAA ATTN: AMXSY-D AMXSY-MP, H. Cohen
	Cdr, USATECOM ATTN: AMSTE-TO-F
	Cdr, CRDC, AMCCOM ATTN: SMCCR-RSP-A SMCCR-MU SMCCR-SPS-IL

USER EVALUATION SHEET/CHANGE OF ADDRESS

This Laboratory undertakes a continuing effort to improve the quality of the reports it publishes. Your comments/answers to the items/questions below will aid us in our efforts.

1. BRL Report Number _____ Date of Report _____

2. Date Report Received _____

3. Does this report satisfy a need? (Comment on purpose, related project, or other area of interest for which the report will be used.) _____

_____

_____

4. How specifically, is the report being used? (Information source, design data, procedure, source of ideas, etc.) _____

_____

_____

5. Has the information in this report led to any quantitative savings as far as man-hours or dollars saved, operating costs avoided or efficiencies achieved, etc? If so, please elaborate. _____

_____

_____

6. General Comments. What do you think should be changed to improve future reports? (Indicate changes to organization, technical content, format, etc.)

_____

_____

_____

CURRENT ADDRESS

_____
Name

_____
Organization

_____
Address

_____
City, State, Zip

7. If indicating a Change of Address or Address Correction, please provide the New or Correct Address in Block 6 above and the Old or Incorrect address below.

OLD ADDRESS

_____
Name

_____
Organization

_____
Address

_____
City, State, Zip

(Remove this sheet along the perforation, fold as indicated, staple or tape closed, and mail.)

FOLD HERE

Director
U.S. Army Ballistic Research Laboratory
ATTN: SLCBR-DD-T
Aberdeen Proving Ground, MD 21005-5066

NO POSTAGE
NECESSARY
IF MAILED
IN THE
UNITED STATES

OFFICIAL BUSINESS
PENALTY FOR PRIVATE USE, $300

BUSINESS REPLY MAIL
FIRST CLASS PERMIT NO 12062 WASHINGTON, DC

POSTAGE WILL BE PAID BY DEPARTMENT OF THE ARMY

Director
U.S. Army Ballistic Research Laboratory
ATTN: SLCBR-DD-T
Aberdeen Proving Ground, MD 21005-9989

FOLD HERE

END

DTIC

9-86